Integration of Extended MHD and Kinetic Effects in Global Magnetosphere Models: Team Successes & Future Directions

Amitava Bhattacharjee

Center for Heliophysics

Department of Astrophysical Sciences and Princeton Plasma Physics Laboratory

Princeton University

Our Team

Center for Heliophysics, Princeton University/PPPL

- Amitava Bhattacharjee, *PI*, Luca Comisso, Ammar Hakim, Jonathan Ng, and Jason TenBarge*

Space Science Center, University of New Hampshire

- Kai Germaschewski, Joachim Raeder, Liang Wang, and Kris Maynard

Los Alamos National Laboratory

- William Daughton, Ari Le, and Adam Stanier

NASA Goddard Space Flight Center

- Li-Jen Chen, John Dorelli, Alex Glocer, Christopher Bard, and Shan Wang

This is a highly leveraged program, involving faculty, research scientists, postdoctoral fellows, and graduate students. Most participants are supported only partially by the NASA-NSF Collaboration.

Ph. D. Theses: Liang Wang (2014), Lijia Guo (2015), Kris Maynard (2018), Jonathan Ng (2018)

Team meets through monthly telecons, an all-hands meeting at Princeton every Spring, and satellite meetings at the Fall AGU/GEM meetings. Organized Special Session at Fall AGU Meeting.

- Synergisms with astrophysical, fusion and high-energy-density plasma physics

Primary Objective

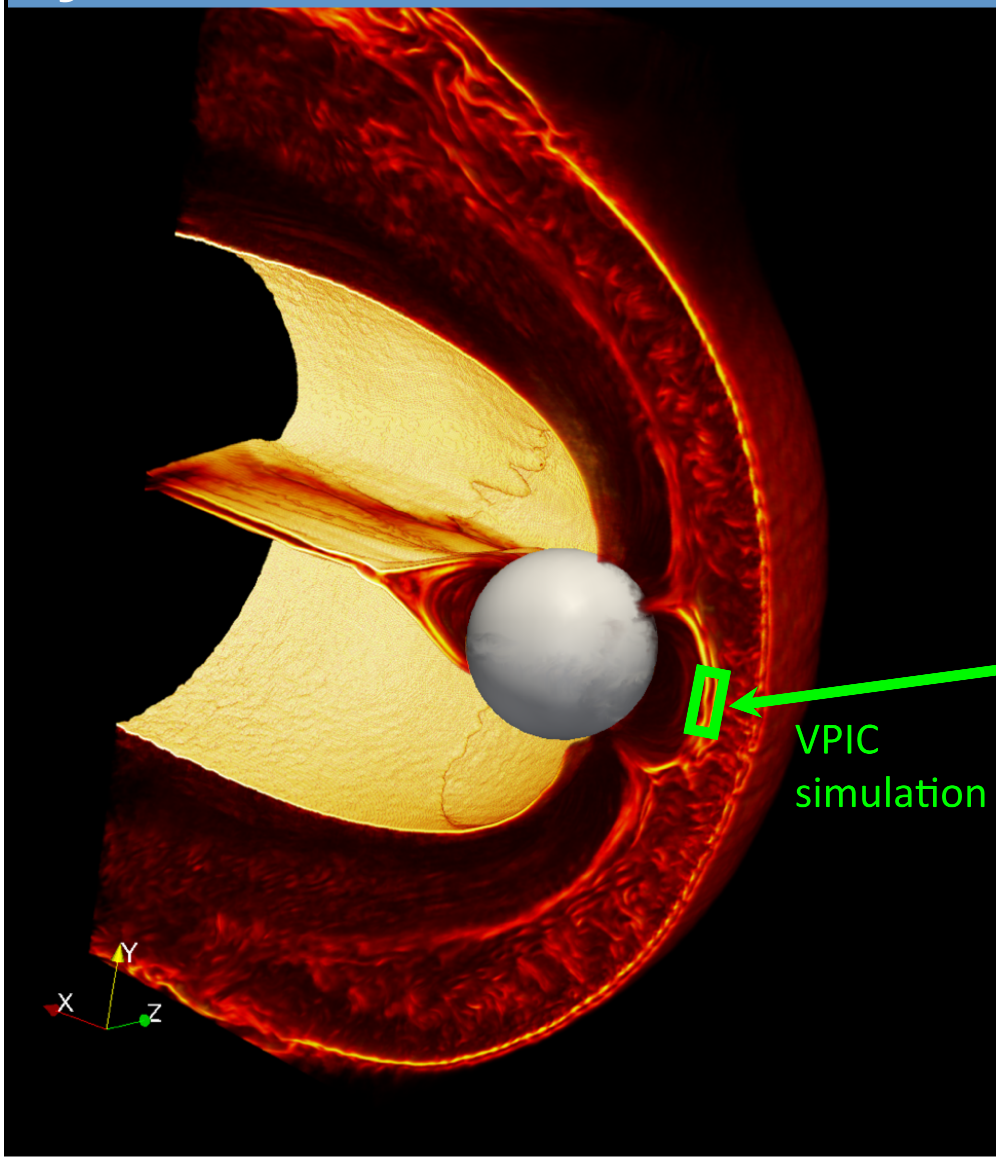
Deliver a global magnetosphere code to CCMC which integrates extended MHD and kinetic effects, with verification and validation with observations.

Today's presentations:

- Integration of Extended MHD and Kinetic Effects into Global Magnetosphere Models: Team Successes & Future Directions : A. Bhattacharjee, *Princeton University*
- Next generation OpenGGCM: K. Germaschewski, *UNH*
- Kinetic Simulations of MMS observations : A. Le, *LANL*

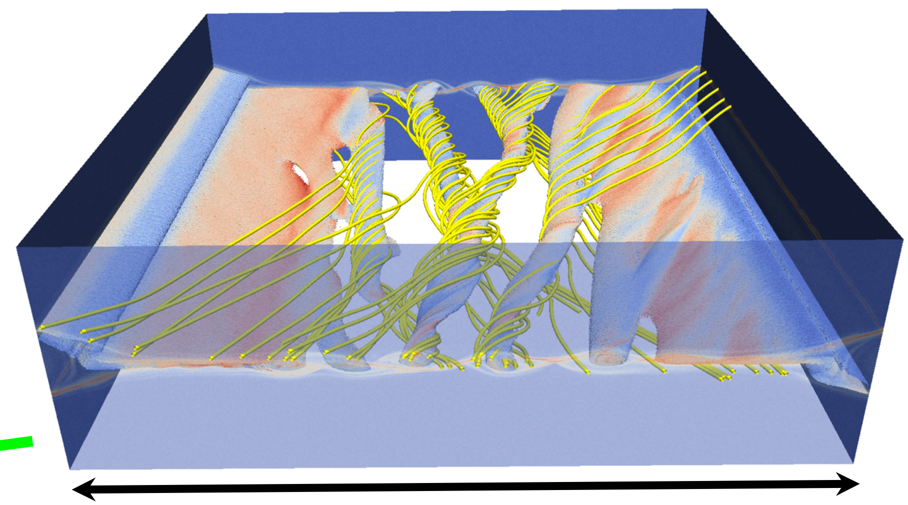
Motivation: What simulations are feasible at the petascale?

Hybrid ~10^{10} cells ~ 10^{12} ions



Fully Kinetic

$\sim 10^{10}$cells $\sim 10^{12}$ particles



$\sim 100 d_i \sim R_E$

$3D \rightarrow m_i/m_e = 100 - 400$

$2D \rightarrow m_i/m_e = 400 - 1836$

Desiderata of Capabilities (as stated in original proposal)

- Capability to study processes occurring at ion and electron scales (but with artificial mass-ratio), including current layers and dissipation regions with scale separation between ions and electrons (done),
- Capability to include new equations of state for the anisotropic and tensor electron and ion pressure, with significant implications for energy, magnetic flux, and particle transport (done),
- Capability to handle multiple ion species (such as hydrogen *and* oxygen), thus enabling the coupled treatment of composition, wave and instability dynamics in the magnetosphere, and its implications for the onset of substorms and storms (done),
- Efficient and flexible computer simulation codes that use state-of-the-art algorithms and scale to up to tens of thousands of processors on modern computational architectures (partially done),
- Validation and verification plan to model geospace that can be tested with spacecraft observations (partially done, primarily in the context of MMS) ,
- Deliverable to NASA CCMC for community access (some modules have been delivered, some are under way).

And more…..

Suite of Codes

- Next Generation OpenGGCM (K. Germaschewski and J. Raeder, *Leads*): *OpenGGCM 4.0 is already available in CCMC and presently under use by community*
- *OpenGGCM 5.0 (including Rice Convention Model to CCMC, Summer 2017)*

  Next Generation OpenGGCM will be made available in Fall, 2017.
- Gkeyll: Testbed for testing equation of state closures in multi-fluid formulation (A. Hakim, *Lead*) (***Breakthrough****, not anticipated at the time of writing of the original proposal*)

  Open source: https://bitbucket.org/ammarhakim/gkeyll

  SimJournal: Complete and open journal for simulation use cases.
- Fully Kinetic Codes VPIC (W. Daughton, *Lead*) and PSC (K. Germaschewski, *Lead*): *both Open Source*
- Multiple Ion Species: KepWOM (*delivered 2017*) (A. Glocer, *Lead*)
- Verification and validation with MMS observations (L.-J. Chen and J. Dorelli, *Leads*).

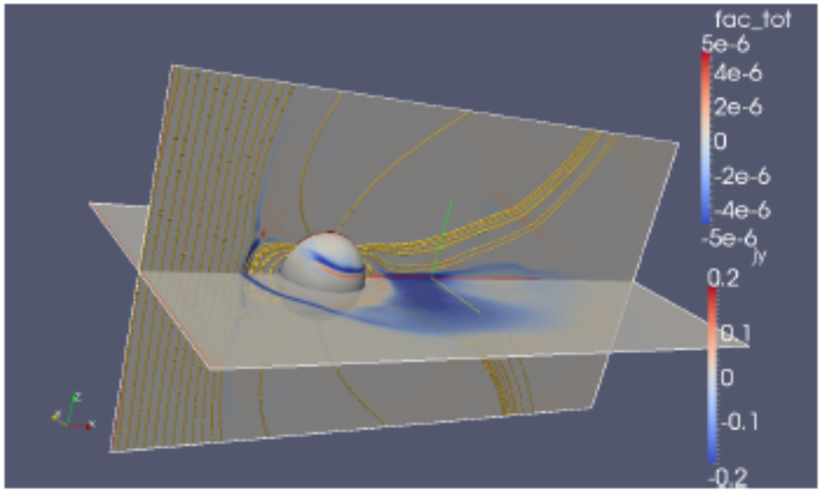
PSC/Gkeyll and VPIC have won DOE ALCC/INCITE grants for high-performance computing (~150 million CPU hours/year on Titan at ORNL).

Our Science Strategy

- Develop kinetic closure relations from first-principles theory: (i) 5-moment, (ii) 10-moment, and (iii) 20-moment extensions
- Test closure formulations through challenge problems in GKEYLL: (1) The Ganymede problem, (2) The island coalescence problem. Compare the results of GKEYLL with PIC simulations. *(Problem 2 has led to the surprising discovery on the importance of ion kinetics, not foreseen in the original proposal*.)
- Couple GKEYLL and OpenGGCM
- Verification with other codes, and validation with MMS data

Our deliverable

Next generation OpenGGCM



- Options for fluid plasma models (MHD, Hall-MHD, multi-fluid, pressure tensor closures)
  Adaptive mesh refinement
- Implicit time integration
- Coupled to CTIM (done),
- IPE (in progress), RCM (done).

New components available as open source (LGPL), whole model to be delivered to CCMC.

solar wind b.c.	ionosphere b.c.	CTIM	RCM		openggcm
reconstruct	Riemann	divB	MHD	gkeyll	libmrc/mhd
multi-d fields	domain decomp	mesh refinement	I/O		libmrc/base

Gkeyll: Foundations

Multi-fluid models of plasmas are obtained by taking moments of Vlasov equation

Describe *each species* of the plasma as a finite set of moments of the Vlasov equation

$$\frac{\partial f}{\partial t} + v_j \frac{\partial f}{\partial x_j} + \frac{q}{m}(E_j + \epsilon_{kmj} v_k B_m)\frac{\partial f}{\partial v_j} = 0$$

Truncate the resulting moment system by a closure scheme. Evolve the electromagnetic fields with Maxwell equations, retaining displacement currents.

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0,$$

$$\mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = -\mu_0 \mathbf{J}$$

Sequence of models with 5, 10 and 20 moments

Taking moments of Vlasov equation leads to the *exact* moment equations listed below

$$
\begin{aligned}
\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_j}(n u_j) &= 0 \\
m\frac{\partial}{\partial t}(n u_i) + \frac{\partial \mathcal{P}_{ij}}{\partial x_j} &= nq(E_i + \epsilon_{ijk} u_j B_k) \\
\frac{\partial \mathcal{P}_{ij}}{\partial t} + \frac{\partial \mathcal{Q}_{ijk}}{\partial x_k} &= nq u_{[i} E_{j]} + \frac{q}{m}\epsilon_{[ikl}\mathcal{P}_{kj]} B_l \\
\frac{\partial \mathcal{Q}_{ijk}}{\partial t} + \frac{\partial \mathcal{K}_{ijkl}}{\partial x_l} &= \frac{q}{m}(E_{[i}\mathcal{P}_{jk]} + \epsilon_{[ilm}\mathcal{Q}_{ljk]} B_m)
\end{aligned}
$$

In the **five-moment** model, we assume that the pressure is isotropic $P_{ij} = p\delta_{ij}$. For the **ten-moment** model, we include the time-dependent equations for all six components of the pressure tensor, and use a closure for the heat-flux. In the **twenty-moment** model, we evolve all ten components of the heat-flux tensor, closing at the fourth moment.

These models treat all species of plasma on same footing

Unlike asymptotic models like Hall-MHD or resistive MHD, moment models include electron inertia, do not assume quasi-neutrality, include displacement currents, and, in ten-moment model, include self-consistent equations for pressure tensor. Additional species and "streams" for a species, can be added with minimum modifications.

Hall currents, separate pressures equations for electron and ions, diamagnetic (and other) drifts, and FLR effects from pressure tensor are included automatically, and not via an Ohms Law or auxiliary equations.

Coupling between species is only via Lorentz and current sources. Hence, each species and the EM field can be evolved independently, potentially with different algorithms and time-steps.

Five- and ten-moment models differ on how pressure and heat-flux are handled

Ten-moment model retains all six components of the pressure tensor. A self-consistent time-dependent equation is used

$$\partial_t P_{ij} + u_k \partial_k P_{ij} + P_{ij} \partial_k u_k + \partial_k u_{[i} P_{j]k} + \partial_k Q_{ijk} = \frac{q}{m} B_m \epsilon_{km[i} P_{jk]}$$

Square brackets around indices represent symmetrization. For example, $u_{[i} P_{j]k} = u_i P_{jk} + u_j P_{ik}$.

A closure is needed to determine $\partial_k Q_{ijk}$. One could use even higher moments[5], but some forms of higher moment equations have issues of realizability, i.e. may lead to distribution functions that are negative in some parameter space. Problem of closure does not go away.

Five moment model has $5S + 8$ equations, while ten-moment models have $10S + 8$ equations, where S is number of species.

Our presently implemented closure: local as well as non-local Hammett-Perkins (1990)

$$i k_m Q_{ijm}(k) = v_t |k| \tilde{T}_{ij}(k) n_0,$$

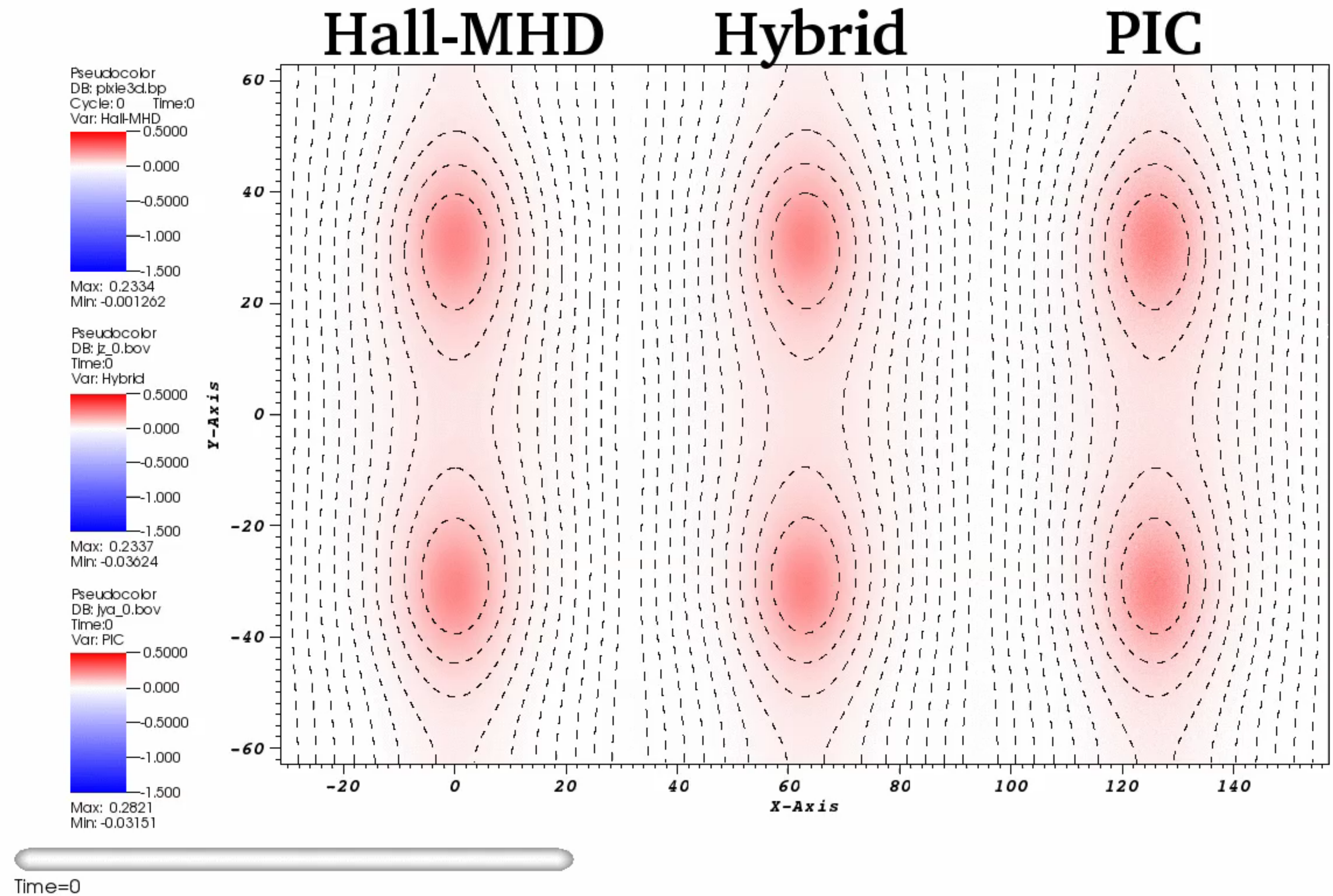
where, now, $k = |\mathbf{k}|$, $\tilde{T}_{ij}(k) = (\tilde{P}_{ij}(k) - T_0 \tilde{n} \delta_{ij})/n_o$

Gkeyll is a C++/Lua package for solution of both (gyro)kinetic as well as multi-fluid equations

Gkeyll was initiated as a project to implement continuum algorithms for the 5D gyrokinetic equations, using discontinuous Galerkin scheme.

- Gkeyll is written in C++ and inspired by framework efforts like Facets, VORPAL (Tech-X Corporation) and WarpX (U. Washington).
- Provides a generic mechanism for implementing solvers, and flexibly composing these to do simulations.
- Programming language Lua, used in widely played games like World of Warcraft, is used as an embedded scripting language to drive simulations.
- MPI is used in parallelization, and HDF5 is used for I/O via txbase library developed at Tech-X.
- A sophisticated meta-build system (developed at Tech-X) is used, and code is version controlled with Mercurial, hosted at www.bitbucket.org.

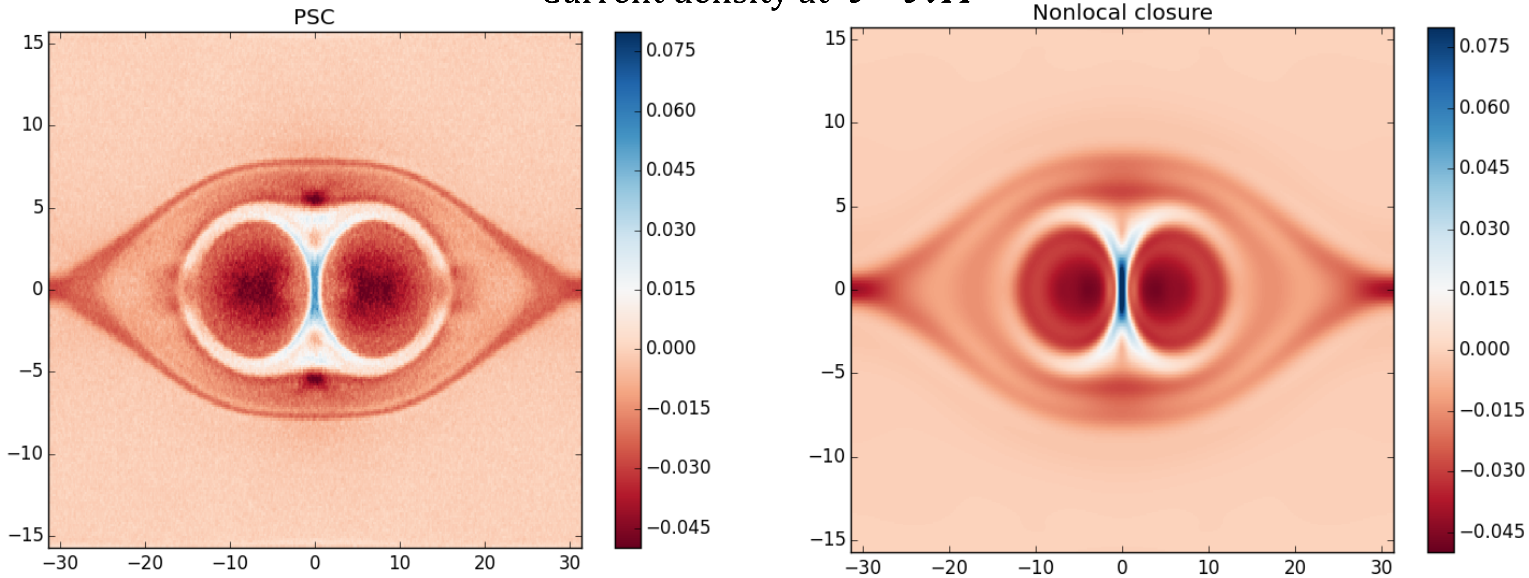
Use of Lua means there is no top-level "main" in the C++ code. Gkeyll is mainly a library, with a simple entry point to load the Lua script, pass it to the interpreter to run. Should allow relatively easy use in other codes.


Hall-MHD
Hybrid
PIC
Pseudocolor
DB: pixie3d.bp
Cycle: 0 Time:0
Var: Hall-MHD
0.5000
0.000
-0.5000
-1.000
-1.500
Max: 0.2334
Min: -0.001262
Pseudocolor
DB: jz_0.bov
Time:0
Var: Hybrid
0.5000
0.000
-0.5000
-1.000
-1.500
Max: 0.2337
Min: -0.03624
Pseudocolor
DB: jya_0.bov
Time:0
Var: PIC
0.5000
0.000
-0.5000
-1.000
-1.500
Max: 0.2821
Min: -0.03151
Y-Axis
60
40
20
0
-20
-40
-60
-20
0
20
40
60
80
100
120
140
X-Axis
Time=0

Nonlocal closure results – island coalescence challenge problem

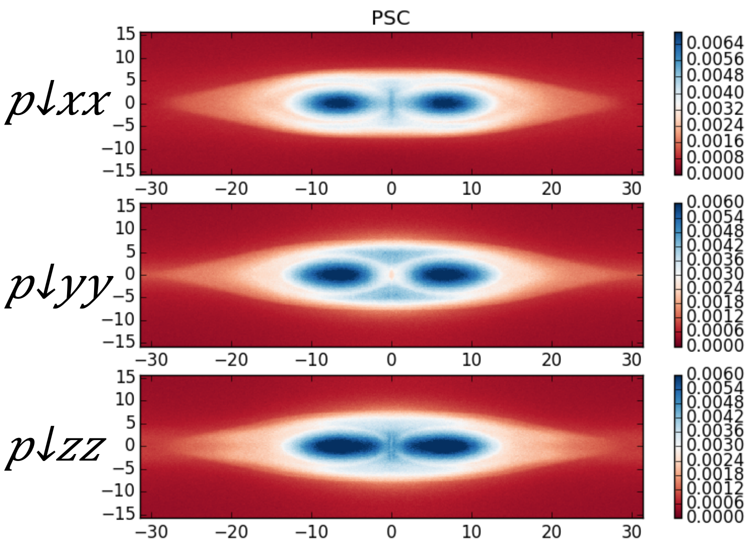
- 2-d model of "self-driven" reconnection
- Ion physics is important in setting the reconnection rate [Stanier 2015]
- *No* adjustable parameters in this study when we use the nonlocal closure of Hammett-Perkins.

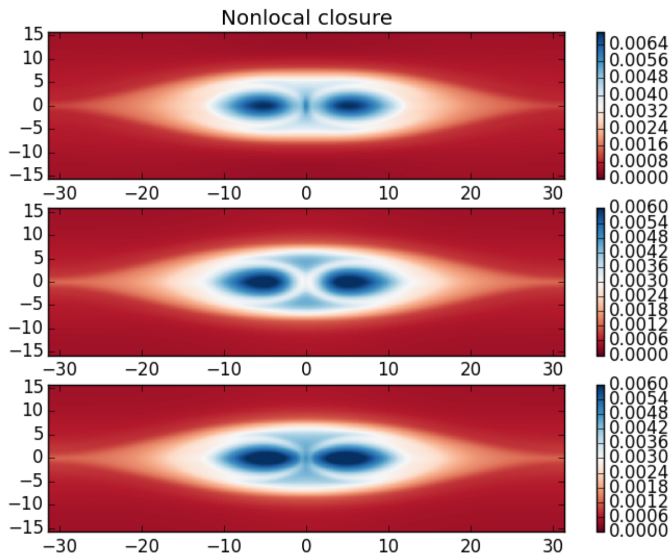
Current density at $t = t_A$



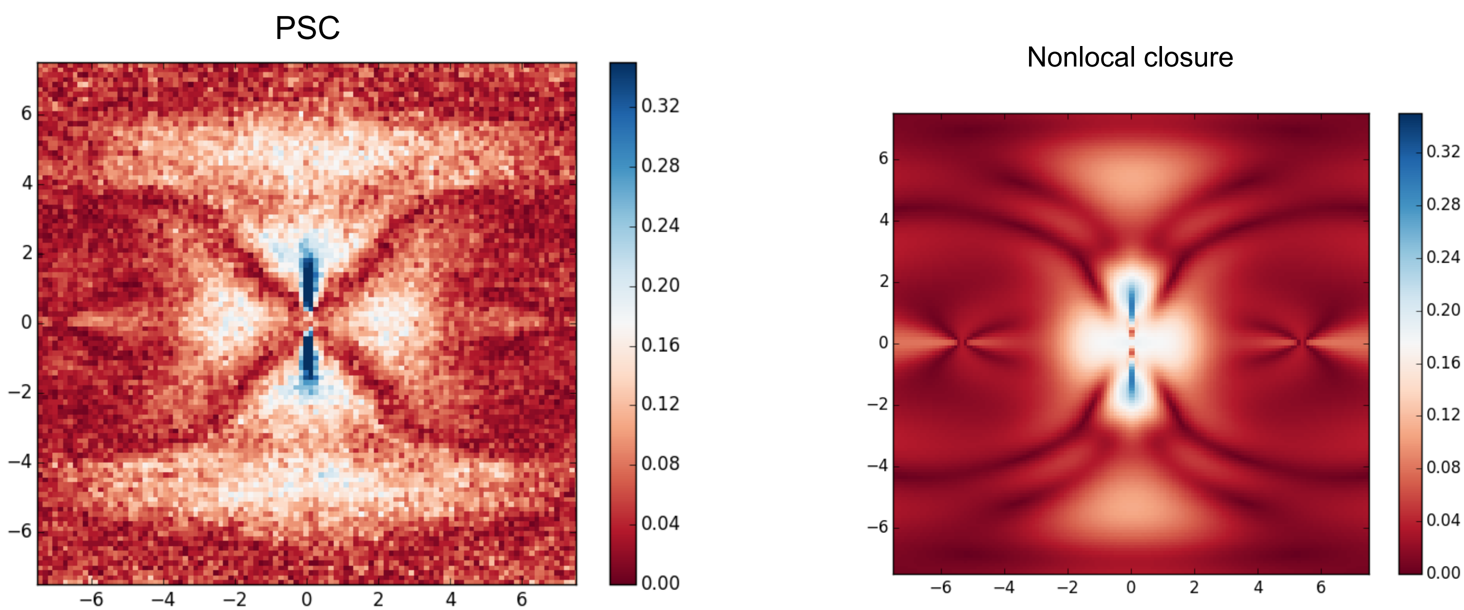
Diagonal components of ion pressure

- Heat flux at the x-point is crucial for better agreement with PIC

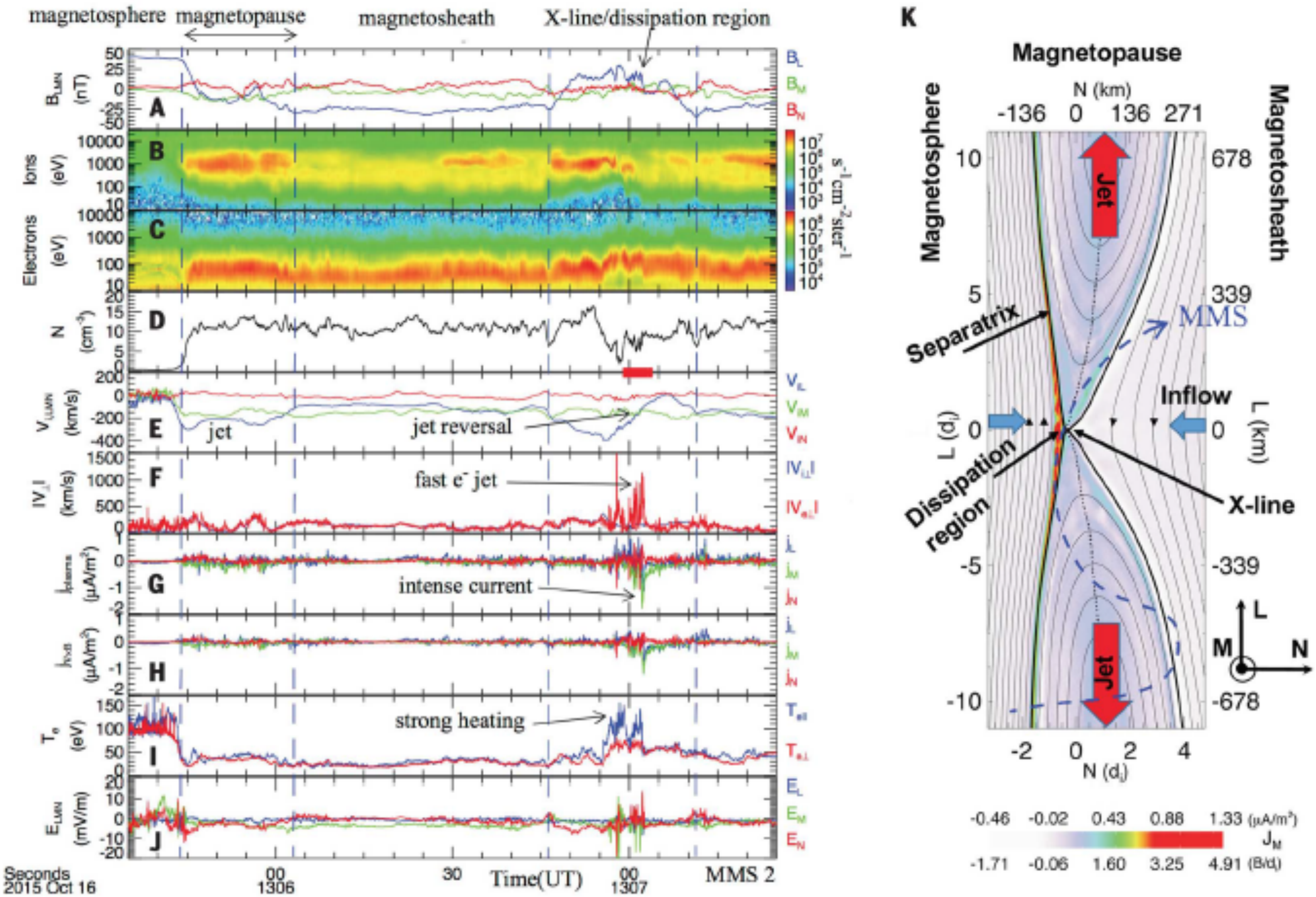




Ion agyrotropy – nonlocal closure shows good agreement



Burch et al (2016) MMS Observations

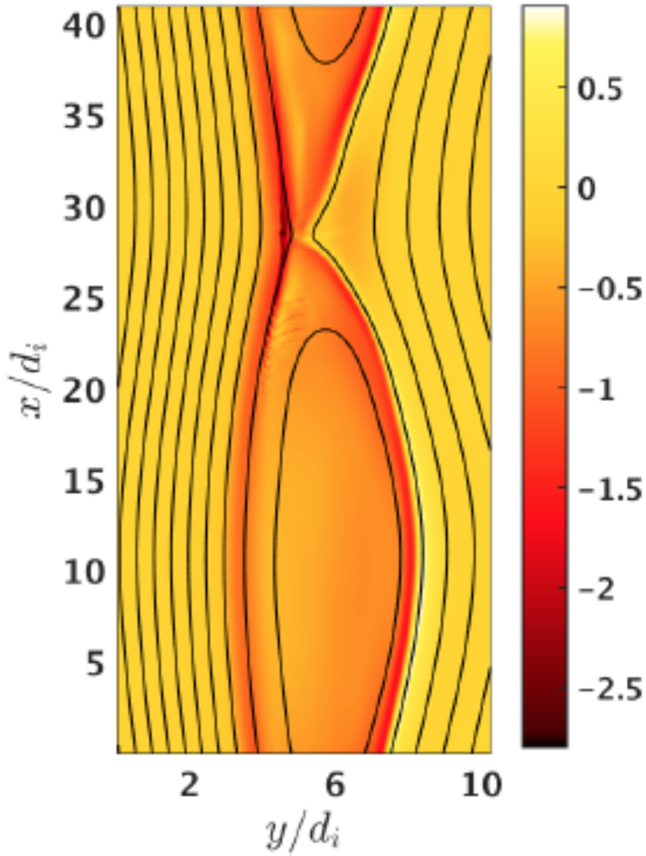


Initial Conditions

$B_g = 0.099$
$w_0 = 1d_{i2}$

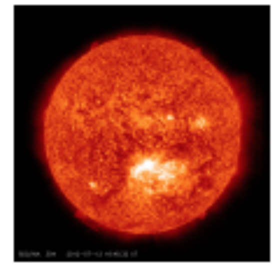
Magnetosphere

$n_1 = 0.06$
$\delta B_1 = 1.696$
$T_{i1} = 7.73$
$T_{e1} = 1.288$
$\beta_{i1} = 0.32$



Magnetosheath

$n_2 = 1$
$\delta B_2 = 1$
$T_{i2} = 1.374$
$T_{e2} = 0.105$
$\beta_{i2} = 1.17$



J. Tenbarge

Dim	m_i/m_e	$\Delta x/d_{e2}$	c/v_{A2}
2D	100	0.2	25
2D	400	0.4	50
2D	1836	0.4	100
3D	100	0.4	25

The 3D run is seeded with noise with RMS amplitude $\delta B_{noise} \sim 0.0005 \delta B_2$.

10 Moment Two Fluid Model

Exact moment equations:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_j}(nu_j) = 0, \qquad \mathcal{P}_{ij} \equiv m \int v_i v_j f d\mathbf{v},$$

$$m\frac{\partial}{\partial t}(nu_i) + \frac{\partial \mathcal{P}_{ij}}{\partial x_j} = nq(E_i + \epsilon_{ijk} u_j B_k), \qquad \mathcal{Q}_{ijk} \equiv m \int v_i v_j v_k f d\mathbf{v}.$$

$$\frac{\partial \mathcal{P}_{ij}}{\partial t} + \frac{\partial \mathcal{Q}_{ijk}}{\partial x_k} = nqu_{[i}E_{j]} + \frac{q}{m}\epsilon_{[ikl}\mathcal{P}_{kj]}B_l. \qquad \mathcal{Q}_{ijk} = Q_{ijk} + u_{[i}\mathcal{P}_{jk]} - 2nmu_i u_j u_k$$

Ten moment closure:

$$\tilde{q}(k) = -n_0\chi_1 \frac{2^{1/2}}{|k|} ikv_t \tilde{T}(k)$$

Three pole Pade approximate of plasma response function

Local approximation of Hammett & Perkins (1990)

$$\partial_k Q_{ijk} \simeq v_t |k_0| (P_{ij} - p\delta_{ij})$$

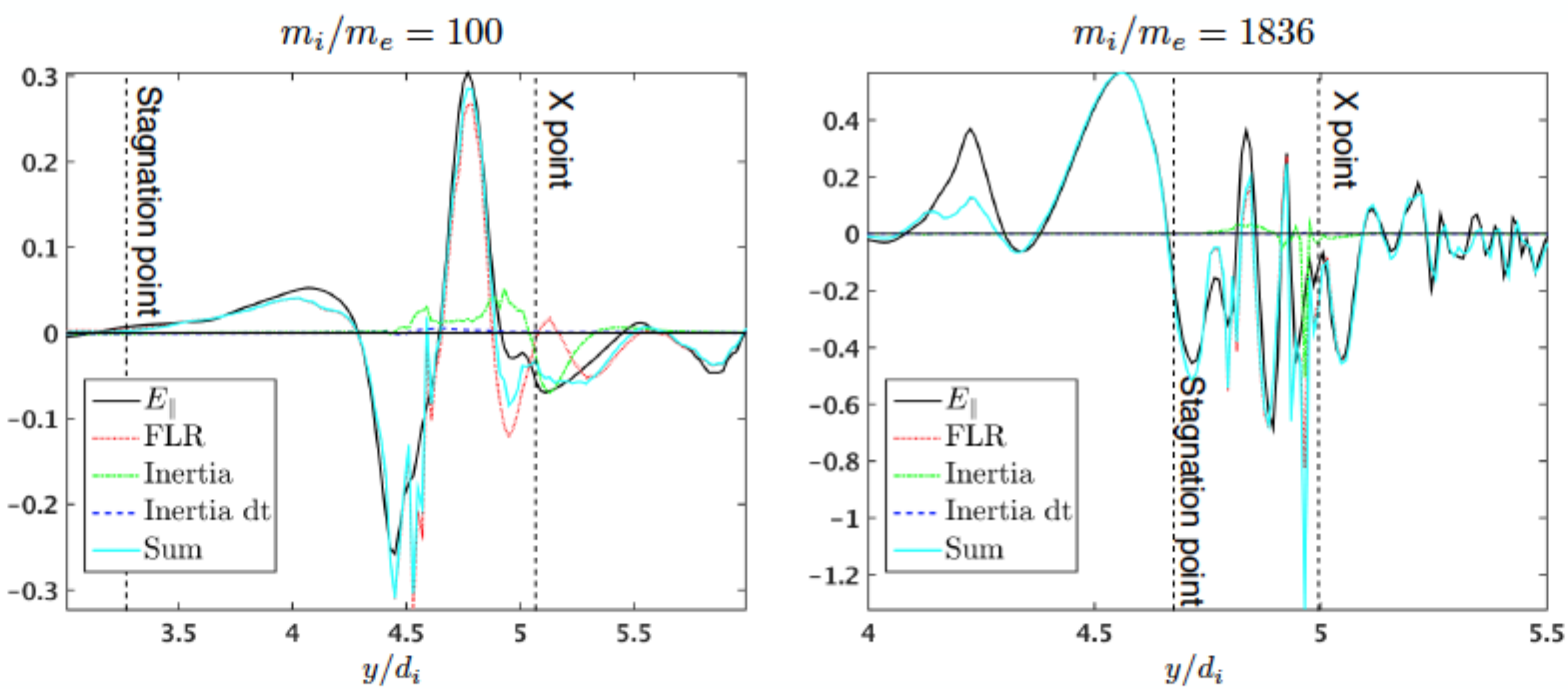
$v_t|k| \sim \nu$ is similar to collisional relaxation to isotropy, where k sets the physical scale at which pressure agyrotropy enters. This closure is intended to mimic Landau damping at small scales.

We will use $k_{0i} = 1/10d_i$ and $k_{0e} = 1/10d_e$, permitting agyrotropy to develop at appropriate scales

Ohm's Law in 2D, Cuts Through the X Point

$$E_\parallel = \mathbf{E}\cdot\mathbf{b} = -\cancel{(\mathbf{u}_e\times\mathbf{B})\cdot\mathbf{b}} - \underbrace{\frac{1}{n_e|e|}(\nabla\cdot P_e)\cdot\mathbf{b}}_{\text{FLR}} - \underbrace{\frac{m_e}{n_e|e|}\left[\nabla\cdot(n_e\mathbf{u}_e\mathbf{u}_e)\right]\cdot\mathbf{b}}_{\text{Inertia}} - \underbrace{\frac{m_e}{n_e|e|}\frac{\partial}{\partial t}(n_e\mathbf{u}_e)\cdot\mathbf{b}}_{\text{Inertia dt}}$$

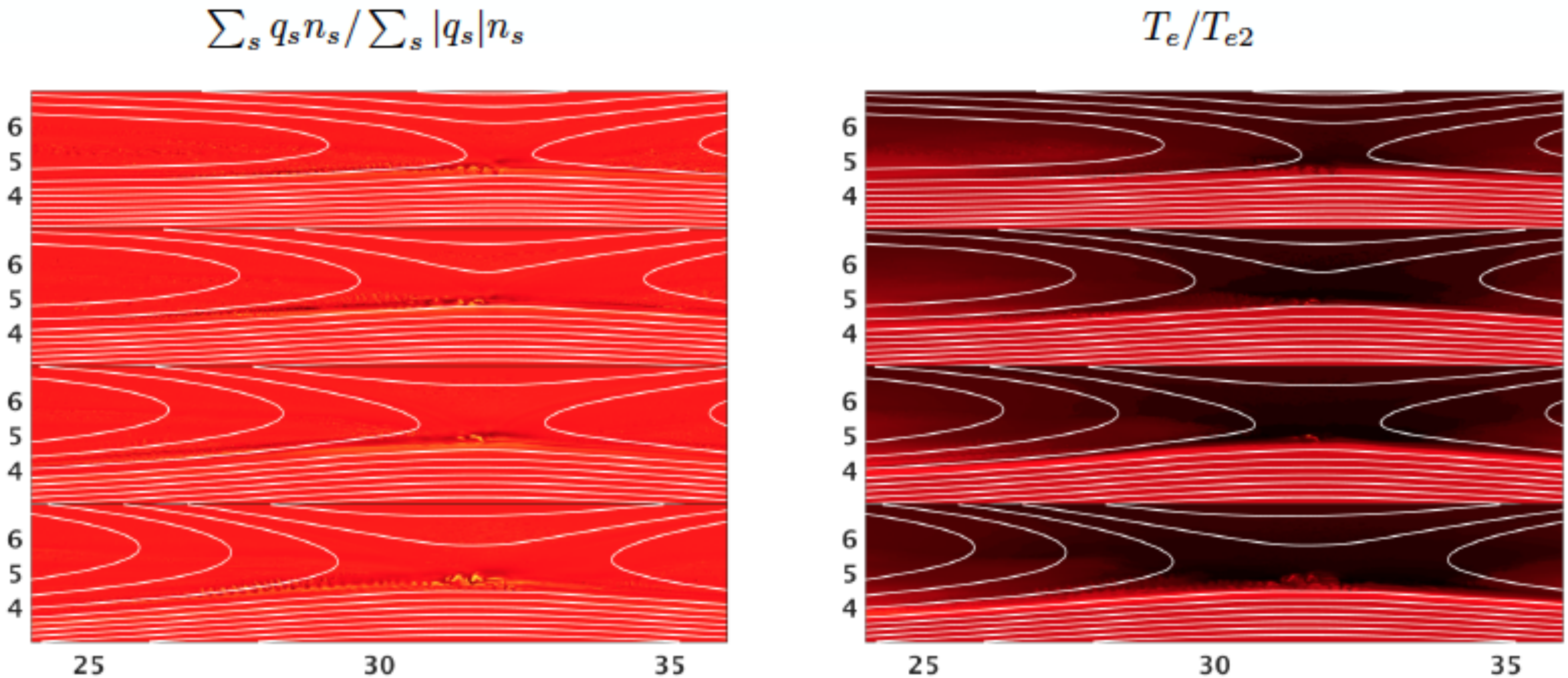
$$t = 30\Omega_{ci}^{-1}$$



Reduced mass ratio runs overemphasize the importance of electron inertia terms in supporting the reconnection electric field

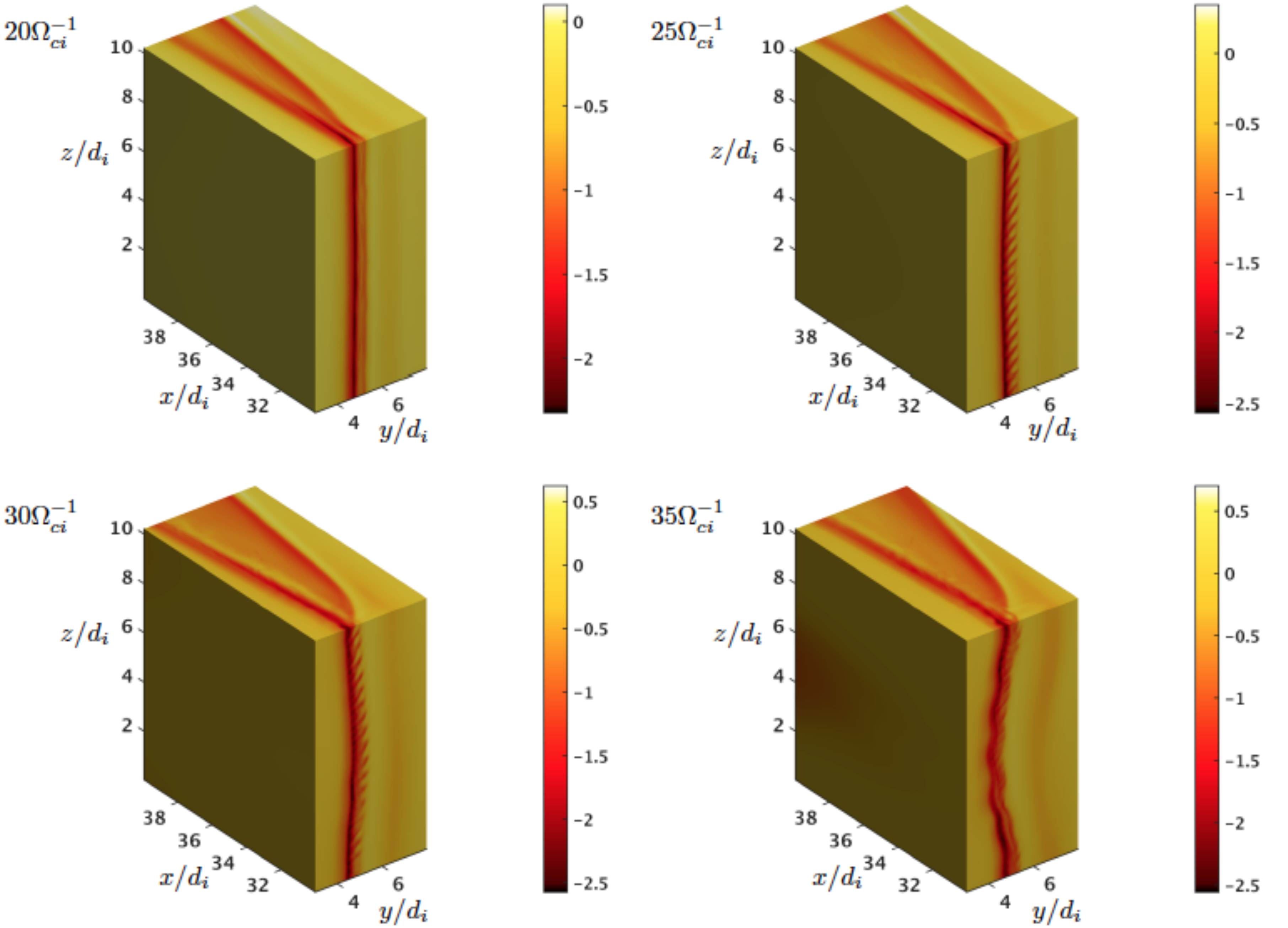
2D Turbulence With A Real Mass Ratio

$$m_i/m_e = 1836$$

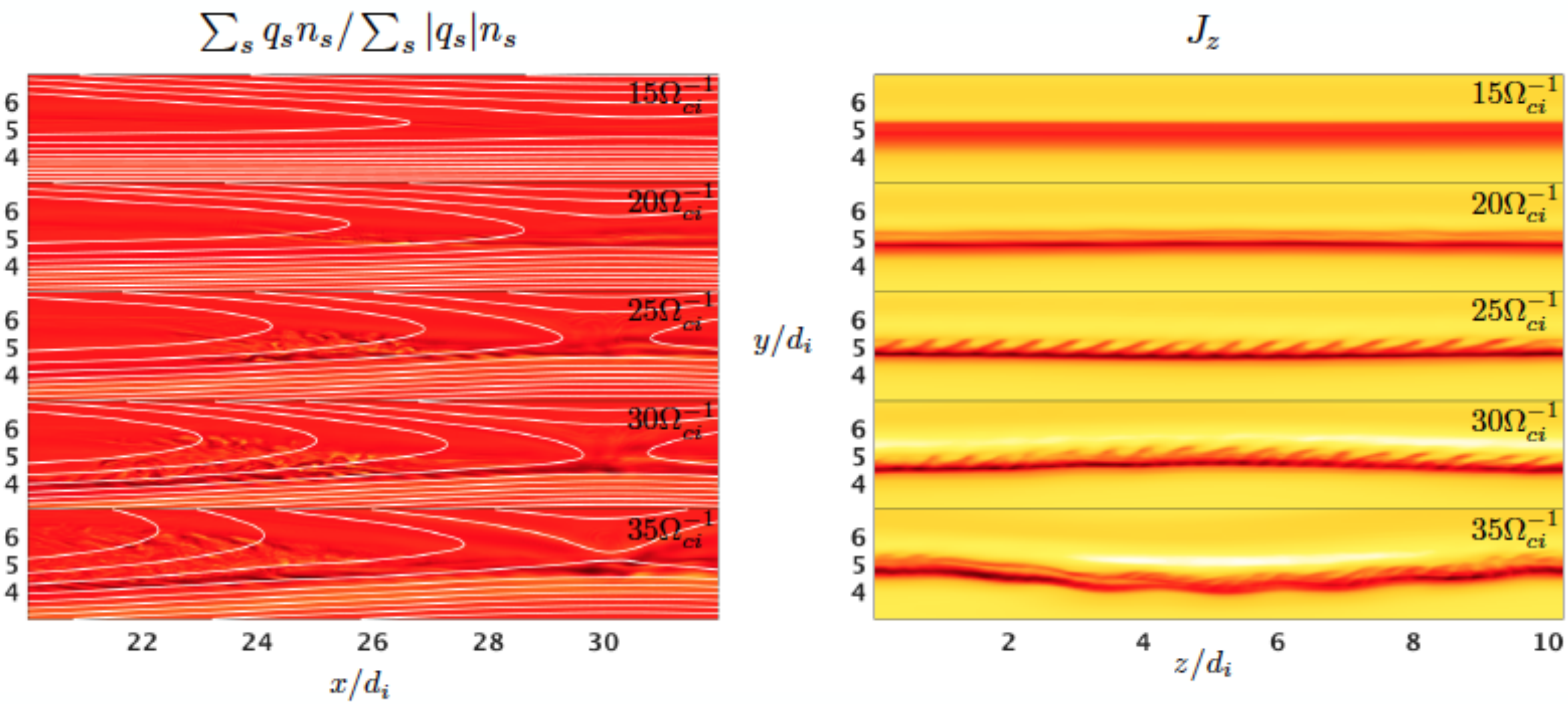


Turbulent eddies have scale $k_x d_e \sim 1$ and scale with $\sim \sqrt{m_i/m_e}$, suggesting electron Kelvin-Helmholtz is driving the turbulence along the separatrix. They also propagate downstream faster, proportional to $\sim \sqrt{m_i/m_e}$.

3D Evolution of Jz



3D Turbulence and Kink Modes



Electron Kelvin-Helmholtz remains apparent in the xy plane but short wavelength LHDI appears to develop in the z-direction at $t\Omega_{ci} \sim 20$ followed by long wavelength LHDI with $k_z \rho_e \sim 1$ and eventually an $m = 6$ kink mode. The short wavelength modes can also be seen to propagate downstream in the xy plane.

The Ganymede Challenge Problem

Ganymede   Mercury   Earth   Jupiter

0.1   0.01   0.005   0.0001

$$\epsilon \equiv \frac{d_i}{L}$$

We expect the extended MHD and kinetic effects to shape the global structure and dynamics of Ganymede's magnetosphere

Overview of 3D simulation Ganymede's magnetosphere

- Ganymede's dipole interacting with southward Jovian magnetic field
- Uses realistic ion mass but artificial electron mass and speed of light
- Correctly captures Alfven wings due to sub-sonic sub-Alfvenic inflow boundary condition
- Demonstrates roles of electrons in both local reconnection physics and global convection

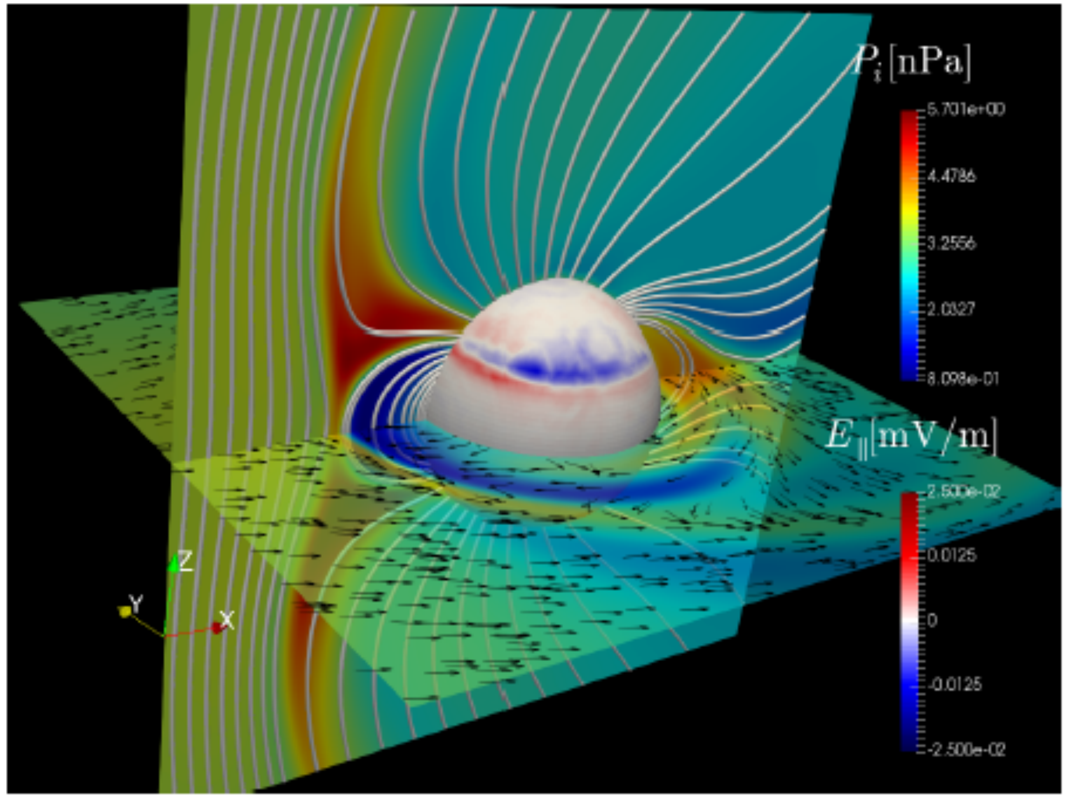
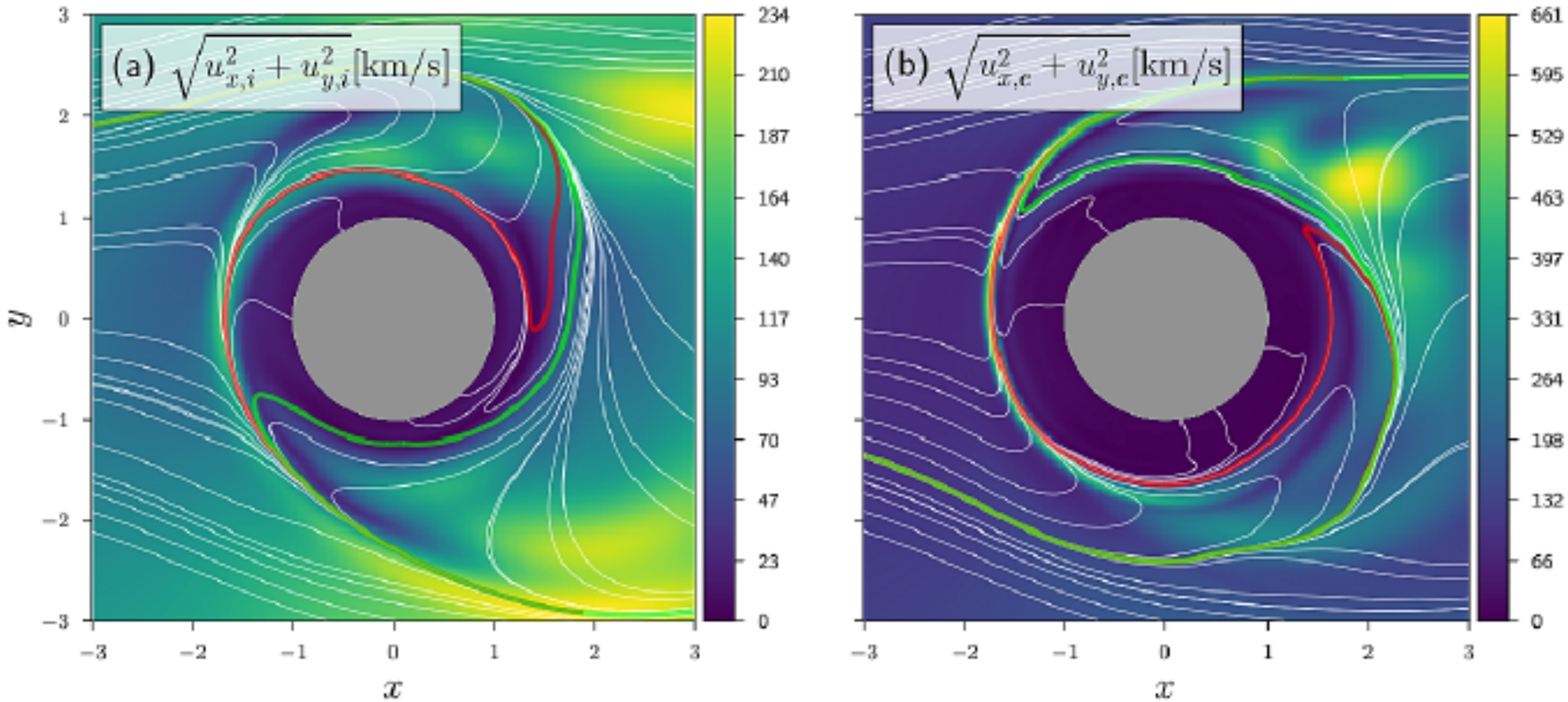


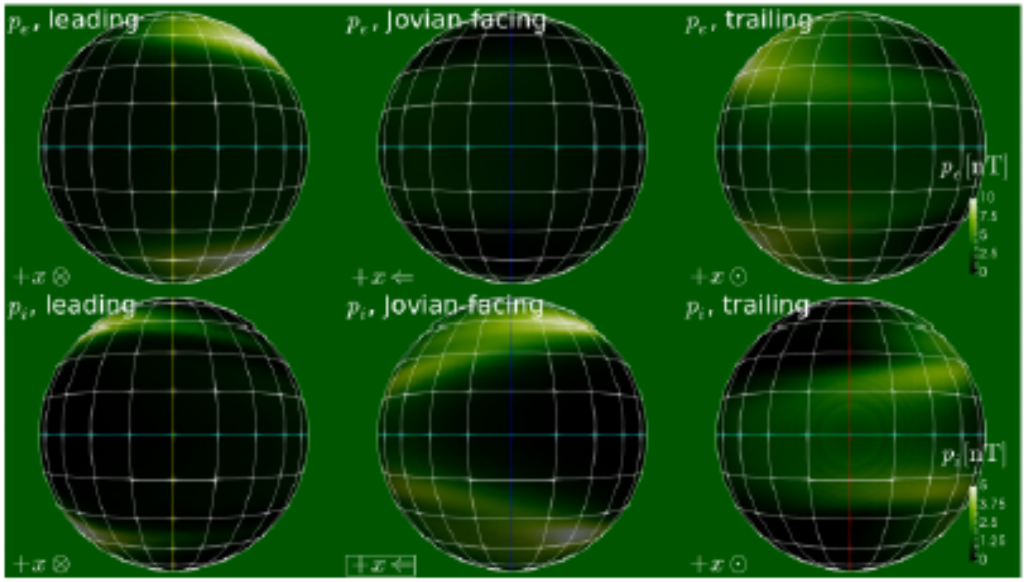
Figure: Snapshot near the Ganymede later in the simulation showing slices of ion pressure, surface parallel electric field, magnetic field lines and ion flow patterns.

Asymmetric drift patterns: equatorial view

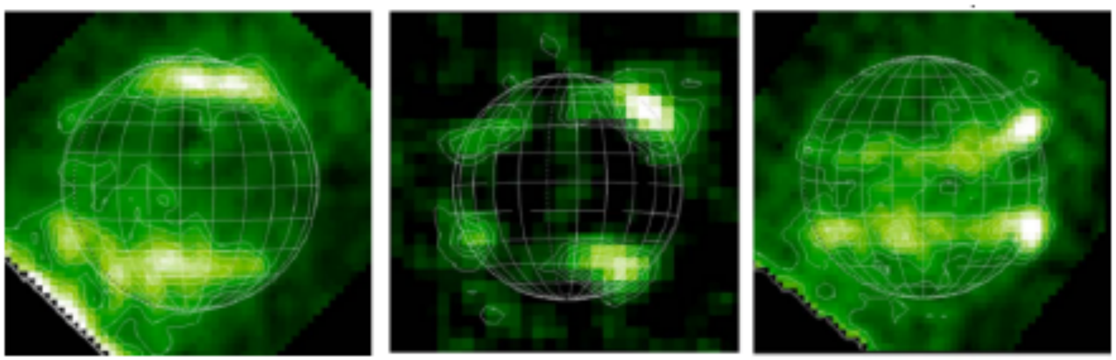


- Jovian plasmas can drift into a inner "magnetosphere"
- electrons and ions follow different paths due to reconnection
- both electron and ion flows can get highly sheared locally

Surface brightness : surface morphology



↑ simulation, pressures ↓oxygen emission from HST (McGrath2013)



- "brightness" represented by surface pressure, not from rigorous semi-empirical models
- captures some key features of observations
- p_e and p_i show different polarities

Summary and Future Plans

- This project requires progress on three major fronts:

(i) development of substantial first-principle theory that is tested by challenge problems in realizing kinetic closures that can be incorporated in fluid models everywhere in the plasma as a uniformly valid approximation.

(ii) Our PIC and XMHD codes, which are Open source, incorporate state-of-the-art algorithms and high-performance computing practices, are ported to multiple platforms (such as GPUs, for the PSC), required by DOE INCITE and ALCC programs.

(iii) GKEYLL mathematical formulation and computational implementation represents a major advance in multi-fluid physics of the magnetosphere. Since it treats all charged particles on an equal footing, it enables straightforward implementation of heavy ions (such as oxygen in the magnetosphere).

Summary and Future Plans (continued)

- Validation with new data from MMS, represents a great opportunity to test reconnection and turbulence physics on electrons and ion scales.

Remark: While our goal is to deliver a global simulation code for space weather applications which includes both electron and ion kinetic physics, the ability or the need to capture all scales is determined by the application at hand. In some global cases, it may be sufficient to capture important ion kinetic scales without resolving electron scales. In all cases, it is very important to recognize what is included, and what is omitted.

Extensive verification, validation, and prediction exercises will be our focus for the next phase of our program. MMS magnetotail program on substorms, provides a great opportunity.

Summary and Future Plans (continued)

- We will deliver both Next Generation OpenGGCM and Gkeyll to CCMC, where the capability of CCMC present computing clusters can be used to make useful runs.
- Gkeyll, VPIC and PSC, while Open Source and with excellent scaling properties, require computational resources well beyond CCMC computing platforms. We will provide a data sets from our CPU-intensive simulations for CCMC archives.
- In 2021, the first exascale computer in the US will be in place (probably in ANL). PPPL has been identified as a hub of the Exascale Computing Program in magnetized plasmas, making use of a software environment for next-generation petascale and exascale computing platforms.
- There is significant room for machine learning algorithms for datasets (from observations as well as computer simulations). NASA is already thinking about some of these issues (work under way by the *Ad Hoc Big Data Task Force*).
- Strategic capabilities should be thought of as participants in the broad context of high-performance computing, and leaders in the realm of space weather. We should build on strong partnerships between NASA, NSF, and DOE, as recommended by the DRIVE initiative. This is a win-win opportunity.